

787,396  
09/288,556

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 13:07:06 ON 12 JAN 2004

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 9 JAN 2004 HIGHEST RN 635758-32-6

DICTIONARY FILE UPDATES: 9 JAN 2004 HIGHEST RN 635758-32-6

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading 787396a.str

L1 STRUCTURE UPLOADED

=>

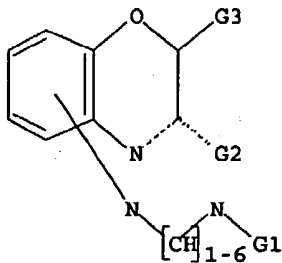
Uploading 787396.str

L2 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 C,H

G2 O,S

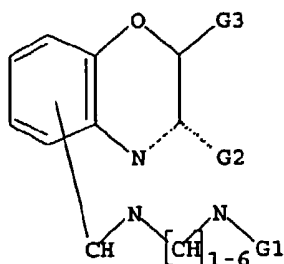
G3 Me,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

Structure attributes must be viewed using STN Express query preparation.

=> d l2

787,346  
09/288,556

L2 HAS NO ANSWERS  
L2 STR



G1 C,H

G2 O,S

G3 Me,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full  
FULL SEARCH INITIATED 13:08:09 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 2008 TO ITERATE

100.0% PROCESSED 2008 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1

=> s l2 sss full  
FULL SEARCH INITIATED 13:08:18 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 1275 TO ITERATE

100.0% PROCESSED 1275 ITERATIONS 5 ANSWERS  
SEARCH TIME: 00.00.01

L4 5 SEA SSS FUL L2

=> file caplus	SINCE FILE	TOTAL
COST IN U.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	310.84	311.05

FILE 'CAPLUS' ENTERED AT 13:08:25 ON 12 JAN 2004  
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FILE COVERS 1907 - 12 Jan 2004 VOL 140 ISS 3

787.396  
09/288,556

FILE LAST UPDATED: 11 Jan 2004 (20040111/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l4  
L5

2 L4

=> d l5 1-2 ibib abs hitstr

L5 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:798206 CAPLUS

DOCUMENT NUMBER: 135:331432

TITLE: Preparation of aminobenzoxazines and aminobenzothiazines as nitric oxide synthase inhibitors and antioxidants.

INVENTOR(S): Hoelscher, Peter; Jautelat, Rolf; Rehwinkel, Hartmut; Jaroch, Stefan; Suelzle, Detlev; Hillmann, Margrit; Burton, Gerardine Anne; McDonald, Fiona McDougall

PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 33 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

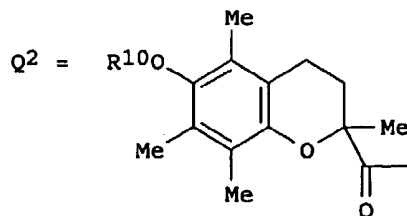
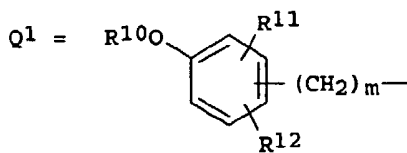
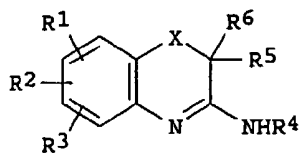
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001081324	A1	20011101	WO 2001-EP4282	20010412
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			

PRIORITY APPLN. INFO.: DE 2000-10021244 A 20000425

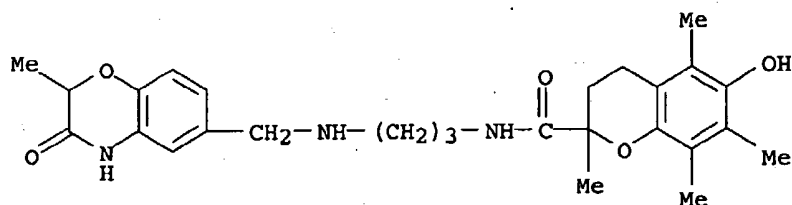
OTHER SOURCE(S): MARPAT 135:331432

GI

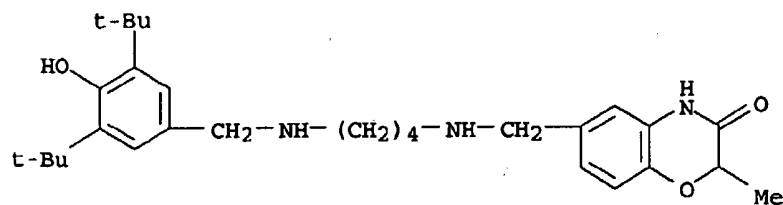


787,396  
09/288,536

- AB Title compds. [I; X = O, S; R1 = (CHR9)nNR7ANR8B, (CHR9)nNR8B, (CHR9)nB; R2 = H; R1R2 = atoms to form a 5-8 membered mono- or bicyclic (unsatd.) ring in which 1 or 2 CH2 groups can be replaced by O or CO, and which is substituted by (CHR9)rNR7ANR8B, (CHR9)nB, or (CHR9)rNR8B; R3 = H, amino; R4 = H, acyl; R5, R6 = H, (substituted) cycloalkyl, Ph, C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl; R7, R8 = H, alkyl, phenylalkyl, alkoxycarbonyl, alkylcarbonyl; A = alkylene, (CH2)pQ(CH2)q; Q = cycloalkyl, indanyl, heterocycloalkyl, aryl, heteroaryl; m, n, p, q, r = 0-6; B = Q1, Q2; R9, R10 = H, alkyl; R11, R12 = H, OH, alkyl, alkoxy], were prepd. as nitric oxide synthase inhibitors and antioxidants (no data). Thus, 6-[N-(4-hydroxy-3,5-di-tert-butylbenzyl)-(tert-butoxycarbonyl)aminomethyl]-2-methyl-2H-1,4-benzoxazin-3(4H)-thione (prepn. given) was stirred 1 day with NH3 in MeOH to give 6-[N-(4-hydroxy-3,5-di-tert-butylbenzyl)-(tert-butoxycarbonyl)aminomethyl]-3-amino-2-methyl-2H-1,4-benzoxazine.
- IT 369650-74-8P 369650-76-0P 369650-79-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. of aminobenzoxazines and aminobenzothiazines as nitric oxide synthase inhibitors and antioxidants)
- RN 369650-74-8 CAPLUS
- CN 2H-1-Benzopyran-2-carboxamide, N-[3-[[[3,4-dihydro-2-methyl-3-oxo-2H-1,4-benzoxazin-6-yl)methyl]amino]propyl]-3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl- (9CI) (CA INDEX NAME)

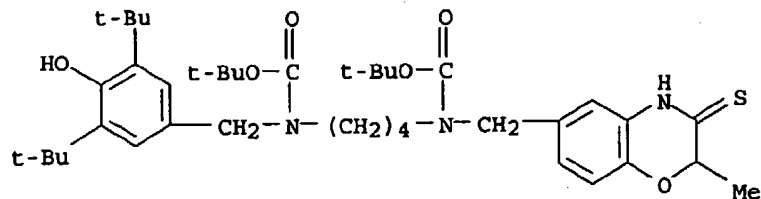


- RN 369650-76-0 CAPLUS
- CN 2H-1,4-Benzoxazin-3(4H)-one, 6-[[[4-[[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]amino]butyl]amino]methyl]-2-methyl- (9CI) (CA INDEX NAME)



- RN 369650-79-3 CAPLUS
- CN Carbamic acid, [[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl][4-[[[3,4-dihydro-2-methyl-3-thioxo-2H-1,4-benzoxazin-6-yl)methyl][(1,1-dimethylethoxy)carbonyl]amino]butyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

787,396  
09/200,556



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:152656 CAPLUS

DOCUMENT NUMBER: 134:193440

TITLE: Preparation of benzoxazines and benzothiazines as nitric oxide synthase inhibitors.

INVENTOR(S): Hoelscher, Peter; Rehwinkel, Hartmut; Jaroch, Stefan; Suelzle, Detlev; Hillmann, Margrit; Burton, Gerardine Anne; McDonald, Fiona McDougall

PATENT ASSIGNEE(S): Schering AG, Germany

SOURCE: PCT Int. Appl., 35 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

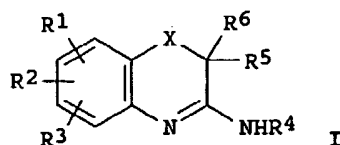
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001014347	A1	20010301	WO 2000-EP8240	20000823
<p>W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM</p> <p>RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG</p>				
DE 19941115	A1	20010301	DE 1999-19941115	19990825
EP 1206458	A1	20020522	EP 2000-962367	20000823
<p>R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL</p>				
JP 2003507460	T2	20030225	JP 2001-518435	20000823
NO 2002000883	A	20020405	NO 2002-883	20020222
PRIORITY APPLN. INFO.:			DE 1999-19941115 A	19990825
			WO 2000-EP8240 W	20000823

OTHER SOURCE(S): MARPAT 134:193440

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09/288,556

- AB Title compds. [I; X = O, S, SO, SO<sub>2</sub>; R<sub>1</sub> = (CHR<sub>9</sub>)nNR<sub>7</sub>ANR<sub>8</sub>B, (CHR<sub>9</sub>)nNR<sub>7</sub>B, etc.; R<sub>2</sub> = H; R<sub>1</sub>R<sub>2</sub> = atoms to form 5-8 membered mono- or bicyclic (unsatd.) (alkyl-substituted) ring substituted by R<sub>1</sub>; R<sub>3</sub> = H, halo, NO<sub>2</sub>, cyano, CF<sub>3</sub>, OCF<sub>3</sub>, SR<sub>9</sub>, OR<sub>9</sub>, cycloalkyl, heteroaryl, COR<sub>14</sub>, (substituted) aryl, alkyl, alkenyl, alkynyl; R<sub>4</sub> = H, acyl; R<sub>5</sub>, R<sub>6</sub> = H, (substituted) cycloalkyl, Ph, alkyl, alkenyl, alkynyl; R<sub>7</sub> = H, alkyl, phenylalkyl, alkoxycarbonyl, alkylcarbonyl; R<sub>8</sub> = H; A = alkylene, alkenylene; B = C:R(CH<sub>2</sub>)pU, C:RNR<sub>15</sub>, SOR<sub>12</sub>, aryloxy carbonyl, benzyloxy carbonyl; R<sub>8</sub>B = 5-7 membered (substituted) heterocyclyl; R = O, S; n, p = 0-6; R<sub>9</sub> = H, alkyl; R<sub>14</sub> = H, OH, alkoxy, Ph, (substituted) alkyl, alkenyl; R<sub>15</sub> = H, alkyl, (substituted) Ph, PhCH<sub>2</sub>], were prepd. as NOS inhibitors (no data). Thus, 6-[[N-(4-chlorobenzyl)pentanethiocarboxamid-6-yl]-(tert.-butyloxycarbonyl)aminomethyl]-3-amino-2-methyl-2H-1,4-benzoxazine.
- IT 327157-36-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(prepn. of benzoxazines and benzothiazines as nitric oxide synthase inhibitors)
- RN 327157-36-8 CAPLUS
- CN 2H-1,4-Benzoxazin-3(4H)-one, 6-[[[(4-aminobutyl)amino]methyl]-2-methyl-, dihydrochloride (9CI) (CA INDEX NAME)

